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MATHEMATICAL PROBLEMS IN MICROMECHANICS AND COMPOSITE MATERIALS

FINAL TECHNICAL REPORT FOR ARO CONTRACT DAAL03-89-K-0039

Robert V. Kohn, Principal Investigator

Marco Avellaneda and Graeme W. Milton, Co-P.I.'s

Courant Institute of Mathematical Sciences

ABSTRACT

This is the final technical report on ARO contract DAAL03-89-K-0039, which began February 1, 1989 and terminated January 31, 1992. The scientific focus of this work is at the frontier where mathematics meets the materials sciences. Physically, we are concerned with the effective moduli of composites, the formation of fine scale structure in coherent phase transitions, and with oscillatory solutions of nonlinear partial differential equations from continuum mechanics. Mathematically, we bring to bear a variety of tools including homogenization, the calculus of variations, and the theory of stochastic processes. Our accomplishments include: (i) new bounds on the effective moduli of two-component and polycrystalline composites; (ii) a new understanding of the role of surface energy in coherent phase transitions; and (iii) rigorous results on the effective diffusivity due to a turbulent velocity field. The training of young scientists, both postdocs and students, has been a major part of our activity.

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I) INTRODUCTION

This is the final technical report on ARO contract DAAL03-89-K-0039, *Mathematical Problems in Micromechanics and Composite Materials*, which began February 1, 1989 and ended January 31, 1992.

The scientific focus of our work is at the frontier where mathematics meets the materials sciences. Physically, we are concerned with issues such as the effective moduli of composites, the formation of microstructure in coherent phase transitions, and the effective diffusivity due to turbulent transport. Mathematically, we bring to bear a variety of tools including homogenization, the calculus of variations, and the theory of stochastic processes.

The scope of this effort is rather broad. It includes static issues such as the effective conductivity of composites and the effective permeability of porous rock. It also includes dynamic issues such as the effective behavior of oscillatory solutions of conservation laws, and an effective law for the transport of a scalar quantity by a turbulent velocity field. Significant recent achievements include the following:

New results on the effective moduli of polycrystalline composites, both in the context of two-dimensional elasticity and in the setting of piezo-electric materials (see Sections II.A and II.B).

A new understanding of the role of surface energy in determining the fine scale structure of twinning due to martensitic phase transitions (see Section III.B).

Rigorous results on turbulent transport, providing the first analytical test of the renormalization-group method introduced by Yakhot and Orzag for modelling the eddy diffusivity due to a turbulent velocity field (see Section IV.A).

There are also many other accomplishments. This report summarizes the most significant ones. A comprehensive list of research papers submitted for publication under this contract appears in Section VI.

While the primary focus of our effort has been on modelling and analysis, numerical simulation has also played a role. One example is our work on elastic polycrystals, which includes a numerical search for sequentially laminated microstructures with extremal effective properties (see Section II.A). Another is our work on structural optimization, which involves the solution of a nonlinear minimization problem (see Section II.C).

The mentoring of postdocs is a major part of our activity. This contract provided approximately 4.5 months of postdoc salary in each academic year. During 1989-90 and 1990-91 these funds supported Weinan E (see Sections IV.B and IV.C); in 1991-2 they supported Kaushik Bhattacharya (see Section III.A). We have also worked closely with other CIMS postdocs, including P. Smereka (Section II.B), G. Allaire (Section II.C), and L. Gibiansky (Section II.A).

We are also active in the training of students. We supervised the thesis research of 7 Ph.D. students who finished their degrees during 1989-90, 1990-91, or will finish in 1991-92. We currently have an

additional 4 students actively involved in research projects. Their work is summarized in Section V. Our ARO contract did not provide academic year support for any of these students, but it did provide two months of summer support for Oscar Bruno (1989), Nick Firoozye (1989), Tami Olson (1990), and Jiang-bo Lu (1991).

For an interdisciplinary effort such as ours to succeed, contact with scientists from the relevant application areas is of paramount importance. We are in close communication with many such individuals, including D. Johnson (Schlumberger Research Lab), P. Sheng (Exxon Research and Engineering), S. Torquato (Physics, North Carolina State), P. Voorhees (Metallurgy, Northwestern), J. Cahn (Metallurgy, NIST), and A. Khachaturyan (Materials Science, Rutgers). Of course, we are also in close contact with the relatively small community of mathematicians working in this area, including Fonseca, Kinderlehrer and Tartar at Carnegie Mellon, James and Luskin at the University of Minnesota, Ball at Heriot-Watt, and Willis at Bath University.

Our ARO-sponsored work is continuing under a new contract, DAAL03-92-G-0011, which began February 1, 1992. Related work is also funded by AFOSR through URI grant no. 90-0090 (Avellaneda, Kohn, Milton), and by NSF through grants no. DMS-9005799 (Avellaneda) and DMS-9102829 (Kohn).

II) EFFECTIVE MODULI OF COMPOSITES

A composite material is by definition a mixture of homogeneous continua on a length scale small compared to that of the loads and boundary conditions, but large enough for continuum theory to apply. Its *effective moduli* describe its overall or macroscopic behavior. Different types of physical behavior lead to different notions of effective moduli. For example, the effective Hooke's law of a linearly elastic composite is a fourth-order tensor relating the average stress to the average strain; the effective permeability of a porous rock is a second order tensor relating the average fluid velocity to the average pressure gradient.

If the microstructure is known exactly, then there is no particular problem in determining the associated effective moduli. In the setting of a linearly elastic composite, for example, the effective Hooke's law σ^* is defined by

$$(\sigma^* \xi, \xi) = \inf_{\langle e(u) \rangle = \xi} \langle \sigma(y) e(u), e(u) \rangle \quad (1)$$

for any second-order tensor ξ . Here $\sigma(y)$ represents the locally varying Hooke's law, which we may take for simplicity to be spatially periodic; u is the locally varying elastic deformation, with linear strain

$e(u) = (\nabla u + {}^t\nabla u)/2$; and $\langle \cdot \rangle$ represents spatial averaging.

If the microstructure is known only approximately, then one might seek to *bound* the effective Hooke's law in terms of whatever is known -- typically the symmetry and two or three-point correlation functions, for a random composite. This is the focus of much of the materials science literature.

Despite its relative maturity as a field of investigation, the study of effective moduli has recently undergone a mathematical renaissance. One reason is a shift of scientific focus. Applications to structural optimization have led to work on the *G-closure problem*, which seeks the precise set of possible Hooke's laws achievable as mixtures of a given set of materials. Also, problems involving physically distinct properties have begun to attract attention, for example the relation between the permeability of porous rock and other properties of the same microstructure. A second reason for the recent surge of activity is the availability of new methods for bounding effective moduli. One is the *translation method*, which modifies a standard variational principle by subtracting a lower semicontinuous quadratic form. Another is the *function space recursion method*, which bounds a linear fractional transformation of the effective tensor instead of the effective tensor itself. A further important development is the use of the construction known as *sequential lamination*, which provides a powerful tool for constructing large classes of composites with explicitly computable effective behavior. We have been exploring these new ideas in a variety of different directions.

II.A) BOUNDS ON EFFECTIVE MODULI

EXTREMAL POLYCRYSTALS

V. Nesi and G. Milton, *Polycrystalline configurations that maximize electrical resistivity*, J. Mech. Phys. Solids 39, 1991, 525-542.

M. Avellaneda, A. Cherkaev, J. Erker, L. Gibiansky, and G. Milton, *work in progress*.

Milton worked with V. Nesi on extremal microstructures for polycrystalline composites in three space dimensions. (A *polycrystal* is a composite composed of a single, anisotropic material mixed with itself in varying orientations.) Prior results of Avellaneda, Cherkaev, Lurie, and Milton had established a lower bound on the effective conductivity of a polycrystal. Milton and Nesi showed that this bound is sharp, for any choice of the basic crystal. The extremal microstructures are interesting, because they have a self-similar microstructure. They were initially discovered numerically, by a search for extremal behavior in the class of all sequentially laminated composites.

Avellaneda and Milton have been working with Erker, Cherkaev, and Gibiansky to identify the precise range of macroscopically isotropic polycrystals, in the setting of two-dimensional linear elasticity. There are two distinct parts to this investigation: Milton and Erker have been exploring the class of polycrystalline composites achievable by "sequential lamination," while Avellaneda, Cherkaev, Gibiansky, and Milton have been exploiting the translation method to prove new bounds. The first part gives an "inner approximation" to the set of all possible composites, while the second part gives an "outer approximation". When they converge, as they do for the case of an orthotropic basic crystal, they give the complete answer.

The work of Erker and Milton is numerical. The main idea is to generate a large number of microstructures by choosing the layering parameters randomly at each stage, an approach first introduced by Nesi and Milton for conductivity. The execution for elasticity is somewhat more complicated, because the elasticity tensor has 6 linearly independent entries. As for the case of conductivity, the extremal microstructures seem to have a self-similar character.

With regard to bounds, Avellaneda and Milton had already obtained optimal bounds on the effective bulk modulus κ^* some time ago, so the main task has been to bound the effective shear modulus μ^* . This has been done using the translation method. The new bounds are achieved by sequential lamination when the basic crystal is orthotropic. Hence in this case the exact class of macroscopically isotropic polycrystals has been identified.

RANDOM POLYCRYSTALS

M. Avellaneda and O. Bruno, *Effective conductivity and average polarizability of random polycrystals*, J. Math. Phys. 31, 1990, 2047-2056.

Avellaneda worked with O. Bruno on the effective conductivity σ^* of a random polycrystal. They considered the case when the orientations of the various grains are statistically independent. If $\sigma_1, \sigma_2, \sigma_3$ are the principal conductivities of the basic crystal, then σ^* is a function of $\sigma_1, \sigma_2, \sigma_3$. They computed the Taylor expansion of σ^* to order 3 about the homogeneous case $\sigma_1 = \sigma_2 = \sigma_3 = 1$. This leads to bounds for σ^* even when $\sigma_1, \sigma_2, \sigma_3$ are far from 1.

NEW METHODS FOR PROVING BOUNDS

G. Milton, *The field equation recursion method*, in Composite Media and Homogenization Theory, G. Dell'Antonio and G. Dal Maso eds, Birkhauser, 1991, pp. 223-245.

G. Milton and K. Golden, *Representations for the conductivity functions of multicomponent composites*, Comm. Pure Appl. Math. 43, 1990, 647-671.

G. Milton, *A brief review of the translation method for bounding effective elastic tensors of composites* in Continuum Models & Discrete Systems, G. Maugin, ed., Longman, 1991, pp. 60-74.

The use of complex function theory to bound effective moduli was developed by D. Bergman and G. Milton in the early 1980's. Its greatest success has been in the setting of the complex dielectric constant of a two-component composite. There have been many attempts to generalize this approach to multicomponent composites, and to other settings such as elasticity. Perhaps the most successful such generalization is Milton's *field equation recursion method*, which uses linear fractional transformations to encode given information (such as volume fractions) in a particularly convenient form. Milton's paper *The field equation recursion method* presented a review of this approach and related ones.

An alternative approach to the multicomponent case is to find a convenient representation of the effective dielectric constant as a function of several complex variables (the dielectric constants of the components). The paper by Milton and Golden takes this viewpoint. It improves on previously available representation formulas by treating the components symmetrically, and by introducing a positive measure whose moments can be determined by perturbation theory around the case of a uniform medium.

Perhaps the most successful of the new approaches for proving bounds is the *translation method*. Milton's article *A brief review...* explains this method in the context of the well-known Hashin-Shtrikman bounds on an isotropic mixture of two well-ordered elastic materials. This expository treatment will help make the translation method more accessible to others in the field.

MIXTURES OF TWO ELASTIC MATERIALS

G. Allaire and R. Kohn, *Optimal bounds on the effective behavior of a mixture of two well-ordered elastic materials*, to appear in Quart. Appl. Math.

G. Allaire and R. Kohn, *Explicit optimal bounds on the elastic energy of a two-phase composite in two space dimensions*, to appear in Quart. Appl. Math.

G. Milton, *Composite materials with negative Poisson's ratio*, to appear in J. Mech. Phys. Solids.

A. Cherkaev, K. Lurie, and G. Milton, *Invariant properties of the stress in plane elasticity and equivalence classes of composites* submitted to Proc. Roy. Soc. London.

During 1986-88 there was major progress on bounds for the effective Hooke's law of a mixture of two well-ordered elastic materials. This resulted from the combined effort of Avellaneda, Kohn, Lipton,

and Milton. The paper *Optimal bounds on the effective behavior...* by Allaire and Kohn presents this theory for the first time in a self-contained, comprehensive, and systematic form. It clarifies a number of points that were known to experts but unclear in the literature. These include: (i) the case when the component materials are anisotropic, (ii) the correspondence between the Hashin-Shtrikman method and the translation method, and (iii) the presentation of the energy bounds as finite dimensional *convex* optimizations. The second paper of Allaire and Kohn, *Explicit optimal bounds ...*, works out the optimal energy bounds explicitly for mixtures of two isotropic elastic materials in two space dimensions.

It was long an open question whether a composite can have Poisson's ratio ν negative, when the component materials have $\nu > 0$. One might have thought not, since essentially all naturally occurring elastic materials (composite or otherwise) have $\nu > 0$. Milton's paper *Composite materials with negative Poisson's ratio* shows that opposite is true: there is in fact no restriction on the effective Poisson ratio, other than the obvious one $\nu > -1$ (which arises from the positivity of the Hooke's law when viewed as a quadratic form on strains). This work highlights the fact that by mixing two commonplace materials in an appropriately chosen microstructure, one can get a composite with bizarre (and possibly useful) effective behavior.

The paper *Invariant properties of the stress...* was motivated by recent work of Day, Snyder, Garboczi, and Thorpe. They observed from numerical experiments that the effective Young's modulus of a two-dimensional perforated composite does not depend on the Poisson's ratio of the matrix. The paper of Cherkaev et al. gives a simple analytical explanation, based on the translation method.

THE ROLE OF SEQUENTIAL LAMINATION

G. Francfort and G. Milton, *Sets of conductivity and elasticity tensors stable under lamination*, in preparation.

G. Milton, *Sets of tensors stable under lamination and quasiconvex translation operators*, in preparation.

K. Clark and G. Milton, *work in progress*.

Milton has been working with K. Clark and with G. Francfort to achieve a better understanding of the role of sequential lamination. Underlying this work is the conjecture, first formulated by K. Lurie and A. Cherkaev, that the set of sequentially laminated microstructures is big enough to "mimic" the behavior of *any* composite material.

There is now a program for confirming this conjecture, based on a newly-discovered link between sequential lamination and quasiconvexity. The link is this: if a set L of effective tensors is closed under

the process of lamination, then for each point x on boundary of L there is an associated quadratic form τ_x , depending only on the second-order behavior of the boundary at x , with the property that τ_x is a quasiconvex quadratic form. Moreover, associated with τ_x there is a set of effective moduli which is stable under homogenization and includes the point x on its boundary. One might hope that as x varies around the boundary of L , these regions would wrap around L , thereby establishing that L is stable under homogenization. (If this were true, it would explain why bounds are always achieved by sequentially laminated microgeometries.) Unfortunately, τ_x does not have this property. However, the choice of τ_x is not unique. Milton is now working on how to adjust it appropriately.

Milton's work with Clark is concerned with the effective conductivity *function* of a two-dimensional conducting polycrystal. Here the effective conductivity is viewed as a tensor-valued function of the principal conductivities of the basic crystal, when the geometry is held fixed. Milton and Clark have shown that the conjecture of Lurie and Cherkaev is valid in this setting in its strongest possible form: every effective conductivity function is achievable by a sequential laminate. This work comprises part of Clark's Ph.D. thesis. It remains an open problem to extend these results to three space dimensions.

II.B) CORRELATION OF PHYSICALLY DISTINCT PROPERTIES

BUBBLY FLUIDS

G. Milton and P. Smereka, *Bubbly flow and its relation to conduction in composites*, J. Fluid Mechanics 233, 1991, 65-81.

Milton and Smereka studied a connection between the effective moduli of composites and the equations of inviscid, bubbly flow. It was recently noted by Wallis that the virtual mass of an arrangement of bubbles is linked to the effective conductivity of a composite with the same microgeometry. Milton and Smereka explored the implications of this relation, especially with regard to the well-posedness (hyperbolicity) of the effective equations governing the flow. Without bubble clustering the equations are ill-posed. When the bubbles group into clusters, however, the equations can become well-posed.

POROELASTICITY

J. Berryman and G. Milton, *Exact results for generalized Gassmann's equations in composite porous media with two constituents*, *Geophysics* 56, 1991, 1950-1960.

Milton and Berryman studied how the elastic properties of porous rock depend on the compressibility of the saturating pore fluid. The situation when the rock is spatially homogeneous was studied long ago by Gassman. His analysis was extended to the heterogeneous case by Brown and Korrington, but their treatment made use of two parameters that depend on the microgeometry of the rock. The new work of Milton and Berryman shows how to evaluate these parameters exactly, when the rock is composed of just two constituents.

PIEZOELECTRIC POLYCRYSTALS

T. Olson and M. Avellaneda, *Effective dielectric and elastic constants of granular piezoelectrics*, *J. Appl. Phys.* 71, 1992 (in press).

M. Avellaneda and T. Olson, *Effective medium theories for piezoelectric composite materials*, to appear in *Recent Advances in Adaptive and Sensory Materials and their Applications*, C. Rogers ed., Technomic Publ. Co.

Avellaneda worked with his student T. Olson on the effective behavior of piezoelectric polycrystals. In such materials, there is a coupling between the electric and elastic fields within each grain. If the composite is macroscopically isotropic then there can be no coupling of the average fields. Nevertheless, the piezoelectric effect is still important in determining the overall dielectric or elastic behavior.

There are essentially three different ways to approach the problem: (i) by using an effective medium theory; (ii) by proving bounds based on statistical hypotheses about the microstructure; and (iii) by proving bounds that are valid without statistical hypotheses on the microstructure. These methods naturally complement one another: (i) and (ii) give answers that are valid for special microstructures, and which may be useful as general rules of thumb; (iii) serves instead to bracket the behavior of any microstructure. These tools have been widely applied in the context of elastic or dielectric polycrystals. Surprisingly, however, there is almost no analogous work on piezoelectric polycrystals. The papers by Avellaneda and Olson extend all three approaches to the setting of piezoelectricity. This work was essentially Olson's Ph.D. thesis.

POROUS ROCK

M. Avellaneda and S. Torquato, *Rigorous link between fluid permeability, electrical conductivity, and relaxation times for transport in porous media*, Phys. of Fluids 3A, 1991, 2529-2540.

M. Avellaneda and S. Torquato, *Cross-property relations for transport in porous media: rigorous link between fluid permeability, conductivity, and relaxation times*, in Multiphase Transport in Porous Media, R. R. Eaton et al. eds., ASME Conf. Proc. 73-81, 1991.

These papers discuss the relation between the effective permeability k of a porous medium (the constant in Darcy's law) and its effective conductivity F (the macroscopic conductivity when the pores are filled with a conducting fluid). Such results are important because one property may be easier to measure than the other. An empirical relation between k and F was recently proposed by Johnson, Koplik, and Schwartz. The work of Avellaneda and Torquato gives an expression for k in terms of the eigenfunctions of the Stokes operator. This leads to rigorous bounds linking k and F , valid for any microstructure. One version of the bounds involves the principal eigenvalue of the diffusion operator (the "diffusive relaxation time"), which can be measured using NMR experiments. The analysis of Avellaneda and Torquato also explains the empirical relation of Johnson-Koplik-Schwartz: it holds when the distribution of the Stokes eigenvalues has a certain form -- a hypothesis which is valid for a broad class of porous media.

II.C) APPLICATION TO STRUCTURAL OPTIMIZATION

SHAPE OPTIMIZATION IN PLANE STRESS

R. Kohn, *Composite Materials and Structural Optimization*, in U.S.-Japan Workshop on Smart/Intelligent Materials and Systems, I. Ahmad et al. eds., Technomic Press, 1990, 272-286.

R. Kohn, *Numerical structural optimization via a relaxed formulation*, to appear in proceedings of NATO-ASI on Free Boundary Problems and Domain Optimization, University of Montreal, July 1990.

G. Allaire and R. Kohn, *Optimal design for minimum weight and compliance in plane stress using optimal microstructures*, in preparation.

Kohn has been working with G. Allaire on the shape optimization of an elastic structure in plane stress, seeking to minimize the work done by a given load ("compliance") subject to a constraint on the total area ("weight"). This is a classic test problem in the optimal design literature. It is usually approached by some version of "front-tracking." That method has the defect of producing output which depends greatly upon the initial guess. In particular, the topology of the "optimal" designs obtained this

way depends significantly on the numerical discretization.

A new approach has emerged in recent years, based on homogenization. The idea is to solve the problem in a "relaxed" formulation, whereby *perforated composite materials* are permitted as structural components along with the originally given material. The essential physical problem is not being changed. However, the relaxed problem has fewer local minima, and it can be discretized without prejudicing the topology of the "optimal" design. The work of Allaire and Kohn solves the compliance optimization problem numerically, demonstrating the practical feasibility of this new approach.

III) VARIATIONAL MODELLING OF PHASE TRANSITIONS

Coherent phase transitions lead to mixtures of different phases or phase variants with characteristic microstructures. It is widely accepted that these microstructures arise due to minimization of elastic energy. A theory of this type was first developed by metallurgists A. Khachaturyan and A. Roitburd using geometrically linear elasticity. A similar but geometrically nonlinear theory has recently been explored by J. Ball and R. James.

This work is closely related to our activity in structural optimization and extremal composites. Roughly, these microstructures arise because Nature is solving an optimal design problem of similar to that discussed in Section II.C We have been exploring this connection, which promises to enrich both theories. We have also been examining the differences between the geometrically linear and nonlinear theories, and the role of surface energy as a selection mechanism.

In some problems, static modelling is not sufficient. Instead one must consider the dynamical process which leads to energy minimization. We have explored one class of such models: interface motion as modelled by the Allen-Cahn equation.

III.A) MICROSTRUCTURE DUE TO ELASTIC ENERGY MINIMIZATION

TWO ELASTICALLY HOMOGENEOUS PHASES

R. Kohn, *The relationship between linear and nonlinear variational models of coherent phase transitions*, in Proc. 7th Army Conference on Applied Mathematics and Computing (West Point, June 1989) ARO report No. 90-1.

R. Kohn, *The relaxation of a double well energy*, Continuum Mechanics and Thermodynamics 3, 1991, 193-236.

Kohn has examined coherent, energy-minimizing mixtures of two elastic phases with different stress-free strains but the same Hooke's laws. This work places the earlier results of Khachaturyan and Roitburd on a sound mathematical basis, and explains the sense in which the theory of Khachaturyan-Roitburd is the geometrical linearization of that of Ball-James.

FINITE VS. LINEAR ELASTICITY

K. Bhattacharya, *work in progress*.

Bhattacharya is undertaking a systematic comparison of the geometrically linear and nonlinear approaches. In some situations they agree not just approximately but even exactly, for example in predicting the directions of twin planes. In other situations the nonlinear theory captures phenomena that the linear one misses entirely, for example the so-called "wedge-like" microstructures in the context of a cubic-tetragonal phase transitions. Besides shedding light on the role of geometrical nonlinearity, this work will make the Ball-James theory more accessible to metallurgists.

III.B) SURFACE ENERGY

BRANCHING OF TWINS

R. Kohn and S. Muller, *Branching of twins near an austenite/twinned-martensite interface*, to appear in Phil. Mag. A.

R. Kohn and S. Muller, *Surface energy and microstructure*, to appear in Shape Memory Materials and Phenomena -- Fundamental Aspects and Applications, C. T. Liu et al. eds., Materials Research Society Proceedings Vol. 246.

Kohn and Muller have studied the role of surface energy in determining the length-scale and fine structure of twinning in martensite. The mathematical essence of the matter is the variational problem

$$\min_{\phi, \gamma = \pm 1} \int_0^1 \int_0^L [\alpha \phi_x^2 + \epsilon |\phi_{yy}|] dx dy + \beta \sum_{k=-\infty}^{+\infty} |k| |\hat{\phi}_0(k)|^2,$$

where ϕ is periodic in y , and we have used the notation

$$\phi(0, y) = \phi_0(y) = \sum_{k=-\infty}^{+\infty} \hat{\phi}_0(k) e^{2\pi i k y}.$$

The discontinuities of ϕ_y represent twin boundaries, while the line $x=0$ represents the austenite/twinned-martensite interface. It turns out that there are two different regimes, depending on the relative values of the parameters α , ϵ , and β . In the first, the twin planes are exactly parallel, and the twin width w is related to the grain size L by the law $w \approx L^{1/2}$. In the second, the twins branch self-similarly as they approach the austenite, and w is related to the distance x to the austenite by the law $w \approx x^{2/3}$. Previous analyses -- of which there are many -- all missed the second regime, though something similar has been noted in the context of ferroelastic domains.

INTERFACE MOTION

L. Bronsard and R. Kohn, *On the slowness of phase boundary motion in one space dimension*, Comm. Pure Appl. Math. 43, 1990, 983-997.

L. Bronsard and R. Kohn, *Motion by mean curvature as the singular limit of Ginzburg-Landau dynamics*, J. Diff. Eqns. 90, 1991, 211-237.

These papers address the "Cahn-Allen equation" $u_t - \epsilon \Delta u + \epsilon^{-1}(u^3 - u) = 0$ in space dimensions $n = 1$ and $n > 1$ respectively. As ϵ tends to 0, the "interfaces" (where $u = 0$) move exponentially slowly when $n = 1$, and they move with normal velocity equal to the mean curvature when $n > 1$. The paper *On the slowness ...* gave a simple, variational argument to explain the former. The paper *Motion by mean curvature ...* gave the first rigorous proof of the latter (in a special, radial setting). Perhaps our greatest accomplishment was to draw attention to this problem, which has since received a lot of mathematical attention.

IV) AVERAGING OF DYNAMICAL PROCESSES

Our research is concerned with physical problems where the quantities of interest are oscillatory. In situations such as turbulent flow, it is not sufficient to consider statics: one must work with evolution equations instead. Avellaneda and E have worked on the averaging of dynamical equations, from somewhat different viewpoints.

Avellaneda's work has been joint with A. Majda. They consider the passive advection of a scalar quantity by a stationary, incompressible velocity field. The basic equation is

$$T_t + u(x) \cdot \nabla T = D \Delta T, \quad T(x, 0) = T_0(\epsilon x), \quad (*)$$

with $u(x)$ a specified random velocity field and ϵ a small parameter. The goal is to identify an effective equation for T in an appropriate long-distance, large-time scaling. The scientific importance of this work lies in its link to recent theories for modelling eddy diffusivity in turbulent flow. In particular, the work of Avellaneda and Majda has provided the first analytical test of the RNG ("renormalization group") method developed by Yakhot and Orszag for estimating eddy diffusivity in fully developed turbulence.

Weinan E has been studying oscillatory solutions of various nonlinear evolution equations from continuum mechanics. Following the lead of B. Engquist, his work has been oriented around the following four basic questions:

- (i) Do oscillations propagate, or are they damped out?
- (ii) Is there an effective equation that describes the weak limit of a family of oscillatory solutions?
- (iii) Can one describe the asymptotic form of the oscillations?
- (iv) Can a numerical scheme yield the correct effective behavior without necessarily resolving the fine scale structure of the oscillations?

IV.A) TURBULENT TRANSPORT

EFFECTIVE EQUATIONS

M. Avellaneda and A. Majda, *Mathematical models with exact renormalization for turbulent transport*, Comm. Math. Phys. 131, 1990, 381-429.

M. Avellaneda and A. Majda, *Homogenization and renormalization of multiple-scattering expansions for Green's functions in turbulent transport*, in Composite Media and Homogenization Theory, G. Dell'Antonio and G. Dal Maso, eds., Birkhauser, 1991, 13-37.

M. Avellaneda and A. Majda, *An integral representation and bounds on the effective diffusivity in passive advection by laminar and turbulent flows*, Comm. Math. Phys. 138, 1991, 339-391.

M. Avellaneda and A. Majda, *Application of an approximate R-N-G theory to a model for turbulent transport with exact renormalization*, in The Dynamical Systems Approach to the Theory of Turbulence in Fluid Flows, C. Foias et al. eds., Springer-Verlag, in press.

M. Avellaneda and A. Majda, *Approximate and exact renormalization theories for a model for turbulent transport*, Phys. Fluids A 4, 1992, 41-57.

M. Avellaneda and A. Majda, *Mathematical models with exact renormalization for turbulent transport II: non-Gaussian statistics, fractal interfaces, and the sweeping effect*, Comm. Math. Phys. 148, 1992 (in press).

M. Avellaneda and A. Majda, *Renormalization theory for eddy-diffusivity in turbulent transport*, submitted to Phys. Rev. Lett.

These papers are concerned with the effective diffusivity due to turbulent flow, as modelled by Eqn.

(*) above. When the Peclet number

$$Pe = \frac{1}{D} \left[\int \frac{\langle |d\hat{u}(k)|^2 \rangle}{|k|^2} \right]^{1/2}$$

is finite, the appropriate scaling is diffusive: $T(\frac{x}{\epsilon}, \frac{t}{\epsilon^2})$ converges as ϵ tends to zero to a limit \bar{T} which solves a diffusion equation

$$\bar{T}_t = D^* \Delta \bar{T}, \quad \bar{T}(x, 0) = T_0.$$

This was proved in *An integral representation and bounds...*, using methods more commonly associated with the theory of composite materials. That paper also explored how statistical information about u leads to bounds for the effective diffusivity D^* , and how D^* can be computed exactly for certain special classes of velocity fields.

When the Peclet number is infinite the situation is different; this phenomenon is called "anomalous diffusion." For infinite Peclet number there is no universal scaling or effective equation; the properties of the velocity field determine the appropriate scaling $T(\frac{x}{\epsilon}, \frac{t}{\rho(\epsilon)})$. The effective equation for the limit \bar{T} may or may not be local. In *Mathematical models with exact renormalization...*, Avellaneda and Majda computed the effective behavior explicitly for several classes of velocity fields with infinite Peclet number. The paper *Homogenization and renormalization ...* gave another approach to the analysis, based on perturbation expansions for the associated Green's functions. These rigorous results were compared to ones obtained using the RNG method of Yakhot and Orszag, in the papers *Application of an approximate R-N-G theory ...* and *Approximate and exact renormalization theories ...*. There are a limited number of possible effective behaviors, which can be viewed as distinct types or "phases" of turbulent behavior. The RNG method misses some of the phases completely, because it is perturbative in character. Where it applies, however, its results are remarkably accurate. The paper *Renormalization theory for eddy diffusivity ...* demonstrates that the phase diagram is not specific to the details of the "exactly renormalizable" examples. The same picture applies for any random, isotropic, incompressible velocity field in a neighborhood of the Kolmogorov-Obukhov regime. The paper *Mathematical models ... sweeping effect* extends this work to the transport of *interfaces* rather than individual particles. Rigorous results are obtained concerning the fractal dimension of an evolving interface, and these are linked to experimental work in the turbulence literature.

SIMULATION

M. Avellaneda, I. Kim, and S. Torquato, *Diffusion and geometric effects in passive advection by random arrays of vortices*, Phys. of Fluids 3A, 1991, 1880-1891.

M. Avellaneda, C. Apelian, and F. Elliott, *work in progress*.

These papers, too, are concerned with the effective diffusivity due to turbulent transport. The one by Avellaneda, Torquato, and Kim addresses the case when u is a shear flow with "random vorticity" and finite Peclet number. One interesting result is that parameters such as the vortex density and vortex strength have a significant effect on the Lagrangian history of a fluid particle, even among velocity fields with the same effective behavior.

For infinite Peclet number, Avellaneda and Majda have obtained analytically explicit results (summarized above) for certain velocity fields of the form $u = (0, 0, u(x_1, x_2))$. More complicated velocity fields must be studied numerically instead. The work of Avellaneda, Apelian, and Elliott is considering velocities of the form $u(x_1, x_2) = (u_1(x_2), u_2(x_1))$ in two space dimensions. Their method is to solve the stochastic differential equation

$$\frac{dX(t)}{dt} = u(X(t)) + \sqrt{2D} \eta(t),$$

where η is a Brownian motion process, using Monte-Carlo techniques. One can show that if $\langle X(t)^2 \rangle \approx t^{1/\alpha}$ then the correct scaling for the PDE is $x \rightarrow x/\epsilon$, $t \rightarrow t/\rho^2(\epsilon)$ with $\rho(\epsilon) \propto \epsilon^\alpha$.

IV.B) CONSERVATION LAWS

OSCILLATORY INITIAL DATA

Weinan E and R. Kohn, *The Initial-Value Problem for Measure-Valued Solutions of a Canonical 2x2 System with Linearly Degenerate Fields*, Comm. Pure Appl. Math. 44, 1991, 981-1000.

Weinan E and H. Yang, *Numerical study of oscillatory solutions of the gas dynamics equations*, Studies in Appl. Math. 85, 1991, 29-52.

Weinan E, *Propagation of oscillations in the solutions of 1D compressible fluid equations*, submitted to Comm. Partial Diff. Eqns.

B. Engquist and Weinan E, *Large time behavior and homogenization of solutions of two-dimensional conservation laws*, to appear in Comm. Pure Appl. Math.

The paper of E and Kohn considers solutions of the 2x2 system

$$v_t + wv_x = 0, \quad w_t + vw_x = 0$$

with oscillatory initial data. This is perhaps the simplest nonlinear system for which oscillations persist as the solution evolves, and for which the characteristics are solution dependent. The main result of the

paper is a proof that a certain "particle method" correctly captures the overall statistics of an oscillatory solution, even when the numerical grid is too coarse to resolve the detailed structure of the oscillations. This is achieved as a consequence of a uniqueness theorem for an appropriately defined "Young-measure valued solution."

The papers *Numerical study ...* and *Propagation of oscillations ...* are concerned with the system of gas dynamics in one space dimension,

$$v_t - u_x = 0, \quad u_t + p_x = 0, \quad \left(\frac{1}{2}u^2 + e\right)_t + (up)_x = 0,$$

where v is specific volume, u is velocity, p is pressure, and e is the internal energy. Here once again the initial data are assumed to be oscillatory. The work with Yang reports on the results of numerical simulations, and presents an asymptotic analysis. The main conclusion is that oscillations in the velocity and pressure die out quickly, while those in the density persist. With this as motivation, the other paper addresses the case when only the density is oscillatory initially. It derives an effective equation, and proves its validity at least until the formation of shocks.

The paper of E and Engquist considers a scalar conservation law in two space dimensions:

$$u_t^\epsilon + f(u^\epsilon)_x + g(u^\epsilon)_y = 0, \quad u^\epsilon(x, y, 0) = u_0(x, y, \frac{x}{\epsilon}, \frac{y}{\epsilon}).$$

If the equation is linear, then of course oscillations can propagate. If it is "sufficiently nonlinear," however, then they cannot. The assertion that oscillations do not propagate is equivalent, by a scaling argument, to the assertion that solutions with regular initial data decay to a constant as t tends to ∞ . E and Engquist prove this assertion, in the presence of a (very weak) nonlinearity condition.

OSCILLATORY EQUATIONS

Weinan E, *Homogenization of scalar conservation laws with oscillatory forcing terms*, to appear in SIAM J. Appl. Math.

Weinan E and D. Serre, *Correctors for the homogenization of conservation laws with oscillatory forcing terms*, submitted to Asymptotic Analysis.

Weinan E, *Homogenization of linear and nonlinear transport equations*, to appear in Comm. Pure Appl. Math.

E's paper *Homogenization of scalar conservation laws ...* considers a scalar conservation law of the form

$$u_t + f(u)_x = \varepsilon^{-1} h(x/\varepsilon).$$

The associated effective equation turns out to be another conservation law, with a different flux function. This paper also proposes and tests a numerical method for capturing average quantities without resolving the fine scale oscillations. Some of these results are established with full rigor in the joint paper with Serre.

The third paper addresses and equation of the form

$$u_t^\varepsilon + \nabla \cdot (a(x, \frac{x}{\varepsilon}) f(u^\varepsilon)) = 0$$

in two space dimensions. Depending on the topological structure of the velocity field a , the homogenized equation can take a variety of forms: it can be the same linear transport equation with the averaged velocity field, or a second order hyperbolic equation, or a nonlocal diffusion equation with memory effects.

IV.C) TRANSITION TO TURBULENCE

THE KOLMOGOROV CASCADE

Weinan E and C.-W. Shu, "Effective equations and the inverse cascade theory for Kolmogorov flows," submitted to Phys. Fluids.

This work offers a new viewpoint on the 2D Kolmogorov flow, a standard (but far from fully understood) model for the transition to turbulence. The equation is

$$u_t + u \cdot \nabla u + \nabla p = \varepsilon \Delta u + \frac{1}{\varepsilon} \begin{bmatrix} \sin \frac{x_2}{\varepsilon} \\ 0 \end{bmatrix}, \quad \nabla \cdot u = 0.$$

The idea is as follows: as $\varepsilon \rightarrow 0$, there will be a valid effective equation so long as there is a true separation of scales, i.e. until turbulence develops. Thus turbulence can be detected by looking for singularity development in the effective equation. Numerical simulation reveals that as this breakdown occurs, the energy spectrum has the k^{-4} decay predicted by Kolmogorov via scaling arguments.

V) STUDENTS

We supervised the theses of the following 7 Ph.D. students who completed their degrees during 1989-90 or 1990-91 or will do so during 1991-2:

(1) Oscar Bruno, *The Effective Conductivity of an Infinitely Interchangeable Mixture*. (October, 1989.)

Advisors: G. Milton and R. Kohn

In 1969, Miller introduced a class of so-called "cell materials." For these materials the two classical perturbation expansions (the first in terms of volume fraction, the second in terms of heterogeneity) are linked. This leads to bounds on the effective moduli of such materials. Bruno's thesis gave a complete and elegant reorganization of Miller's ideas, based on the notion of "infinite interchangeability."

Current position: Georgia Institute of Technology.

(2) Vincenzo Nesi, *Extremal Microgeometries for Polycrystalline Composites*. (October, 1989.)

Advisors: G. Milton and R. Kohn

Prior work of Avellaneda, Cherkaev, Lurie, and Milton had established bounds on the effective conductivity of a conducting polycrystal in three space dimensions. Nesi's thesis explored various classes of microstructures that achieve equality in the bound.

Current position: University of L'Aquila.

(3) Piotr Rybka, *Dynamical Modeling of Phase Transitions in Solids by Means of Viscoelasticity in Many Dimensions*. (October, 1990.)

Advisor: R. Kohn

Rybka's thesis studied the equation of viscoelastodynamics in several space dimensions, for materials with non-elliptic elastic energies. He showed global-in-time existence, and also that certain quantities (such as the stress) decay as t tends to ∞ . For certain energies with "multiple wells", modelling coherent phase transitions, he proved that multiphase equilibria are stable under perturbations that are small in a sufficiently strong topology. This work basically generalized that of Andrews, Ball, and Pego to a multidimensional setting.

Current position: Warsaw University.

(4) Nick Firoozye, *Optimal Translations and Relaxations of Some Multiwell Energies*. (October, 1990.)

Advisor: R. Kohn.

Firoozye's thesis studied the minimization of "multiwell" elastic energies, of the type proposed by Ball and James for modelling coherent phase transitions in crystalline solids. It also addressed a more general issue in the relaxation of variational problems, namely how to apply the new "translation method" optimally. One specific result is a proof of the following assertion: in two space dimensions, a finite number of pairwise incompatible elastic phases cannot be combined to form an essentially stress-free microstructure. (The corresponding problem in three dimensions remains open.)

Current Position: NSF Postdoctoral Fellow (visiting Heriot-Watt University).

(5) Stathis Filippas, *Center Manifold Analysis for a Semilinear Parabolic Equation Arising in the Study of $u_t - \Delta u = u^p$* . (October, 1990.)

Advisor: R. Kohn.

Filippas' thesis applied ideas from center manifold theory to derive refined asymptotics near blowup for the solution of a semilinear heat equation. While the formal analysis is easy and enlightening, the rigorous analysis is quite nonstandard. This is because all the available estimates are in norms with exponentially decaying weights.

Current Position: University of Paris VI.

(6) Tami Olson, *Overall Properties of Granular Piezoelectrics: Bounds and Effective Medium Approximations*. (October, 1991.)

Advisor: M. Avellaneda.

Olson's thesis analyzed the consequences of piezo-electric coupling between electrical and elastic behavior on the overall effective conductivity of a polycrystal.

Current Position: Yale University

(7) Karen Clark, *Characterizing the Possible Conductivity Functions of Composite Materials*. (to be completed June, 1992.)

Advisor: G. Milton

Clark's thesis considers the effective conductivity *function* of a two-dimensional polycrystal. This means one considers the effective conductivity tensor as a function of the ratio σ_1/σ_2 , where σ_1 and σ_2 are the principle conductivities of the basic crystal and the geometry is held fixed. She derives a special continued fraction representation for the general effective conductivity function. Using this, she shows that such a function can always be achieved by a sequentially laminated microstructure (of possibly infinite rank).

Position for 1992-3: University of Michigan.

We are currently supervising the research of the following four additional students:

(a) Pedro Girao (*Advisor: R. Kohn*)

The problem of "motion by mean curvature" has recently received a lot of attention. So has its cousin, "motion by weighted mean curvature," the analogous evolution law associated to an anisotropic surface energy. M. Gurtin and J. Taylor have pointed out that in the extreme case of a "crystalline" surface energy, one is left solving a system of ODE's rather than a PDE. Taylor and her collaborators have been exploring this as a numerical approximation scheme for general motion by weighted mean curvature, however there are as yet no rigorous results. Girao is studying the convergence of this scheme, and the question of how the approximating crystalline energies should be chosen for maximum numerical efficiency.

(b) Jiang-bo Lu (*Advisor: R. Kohn*)

Lu's thesis project is to bring our work on optimal bounds into contact with the metallurgical literature on the shape of coherent precipitates, when the two phases differ in both their elastic moduli and their stress-free strains. He is concentrating on the regime in which the volume fraction of the precipitate is nearly zero. The conventional method for predicting the shape (in the absence of surface energy) is to assume it is an ellipsoid, then minimize elastic energy as the eccentricity varies. One can use Eshelby's theory, because in the low volume fraction limit the interaction of distinct inclusions should be a second-order effect. Analyses of this kind have been done by several authors, including A. Roitburd. The shortcoming of this approach is that it *assumes* the ellipsoidal geometry, and it *assumes* the ellipsoids are far apart in the low volume fraction limit. The new mathematical

theory of optimal bounds will allow us to test the validity of these hypotheses with complete mathematical rigor. We are presently uncertain whether they are valid, or whether the optimal microstructures might actually be different even in the low volume fraction regime.

(c) Yuri Grabovsky (*Advisor: R. Kohn*)

Grabovsky's thesis project is to understand the influence of surface energy as a selection mechanism, when minimizing the elastic energy of a mixture of two isotropic elastic materials. We know the optimal bounds, and we know that they are achieved by sequentially laminated composites. When the average strain is isotropic we also know another class of optimal microstructures, based on the "concentric sphere construction." Both of these constructions require a lot of surface energy. A little-known series of articles by S. Vigdergauz asserts the existence of a third construction, involving periodically arranged inclusions of one phase in a matrix of the other. If correct, this construction will surely be preferred over the others in the presence of a small surface energy. Therefore Grabovsky's attention is currently focussed on reaching a full understanding of Vigdergauz' papers. Mathematically, the goal of this project is to achieve some marriage between the theory of optimal bounds (see Section II.A) and the effect of surface energy as a selection mechanism (see Section III.B). Physically, the goal is to explain the shapes of coherent precipitate inclusions, when surface energy is small compared to elastic energy.

(e) Chris Apelian (*Advisor: M. Avellaneda*)

Apelian is working on Monte Carlo simulation of turbulent transport (see Section IV.A).

VI) LIST OF ARTICLES COMPLETED UNDER THIS CONTRACT

G. Allaire and R. Kohn, "Optimal bounds on the effective behavior of a mixture of two well-ordered elastic materials," to appear in Quart. Appl. Math.

G. Allaire and R. Kohn, "Explicit optimal bounds on the elastic energy of a two-phase composite in two space dimensions," to appear in Quart. Appl. Math.

M. Avellaneda, "Remarks on the homogenization and boundary control of distributed systems," in Proc. 5th IFAC Symposium on Control of Distributed Systems (Perpignan, June 1989).

M. Avellaneda, C. Bardos, and J. Rauch, "Contrôlabilité exacte, homogénéisation, et localisation d'ondes dans un milieu non-homogène," to appear in Asymptotic Analysis.

M. Avellaneda and O. Bruno, "Effective conductivity and average polarizability of random polycrystals," J. Math. Phys. 31, 1990, 2047-2056.

M. Avellaneda, T. Hou, and G. Papanicolaou, "Finite difference approximations for partial differential equations with rapidly oscillating coefficients," RAIRO-MMAN 25, 1991, 693-710.

M. Avellaneda, I. Kim, and S. Torquato, "Diffusion and geometric effects in passive advection by random arrays of vortices," Phys. of Fluids 3A, 1991, 1880-1891.

- M. Avellaneda and F.-H. Lin, "Un theoreme de Liouville pour equations elliptiques avec coefficients periodiques," *Comptes Rendus Acad. Sci. Paris*, 309, I, 1989, 245-250.
- M. Avellaneda and F.-H. Lin, " L^p bounds on singular integrals in homogenization," *Comm. Pure Appl. Math.* 44, 1991, 897-910.
- M. Avellaneda and A. Majda, "Mathematical models with exact renormalization for turbulent transport, *Comm. Math. Phys.* 131, 1990, 381-429.
- M. Avellaneda and A. Majda, "Homogenization and renormalization of multiple-scattering expansions for Green's functions in turbulent transport," in *Composite Media and Homogenization Theory*, G. Dell'Antonio and G. Dal Maso, eds., Birkhauser, 1991, 13-37.
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- M. Avellaneda and T. Olson, "Effective medium theories for piezoelectric composite materials," to appear in *Recent Advances in Adaptive and Sensory Materials and their Applications*, C. Rogers ed., Technomic Publ. Co.
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- Weinan E, "Propagation of oscillations in the solutions of 1D compressible fluid equations," to appear in *Comm. Partial Diff. Eqns.*
- Weinan E, "Homogenization of linear and nonlinear transport equations," to appear in *Comm. Pure Appl. Math.*
- Weinan E, "Homogenization of scalar conservation laws with oscillatory forcing terms," to appear in *SIAM J. Appl. Math.*

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